

Field-induced Kosterlitz-Thouless transition in the $N = 0$ Landau level of graphene

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At the charge neutral point, graphene exhibits a very unusual high resistance metallic state and a transition to a complete insulating phase in a strong magnetic field. We propose that the current carriers in this state are the charged vortices of the XY valley-pseudospin order-parameter, a situation which is dual to a conventional thin superconducting film. We study energetics and the stability of this phase in the presence of disorder.

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The initial experiments of the quantum Hall effect (QHE) in monolayer graphene discovered the quantum Hall plateaus $\sigma_{xy} = 4(N + \frac{1}{2})(e^2/h)$ ($N \in \mathbb{Z}$) at filling factors $\nu = 2\pi\ell_B^2\rho = \pm 2, \pm 6, \pm 10, \dots$ [1]. Here, ℓ_B is the magnetic length, ρ the carrier density measured from the charge neutral point, and the factor of 4 arises from the spin and valley (K and K') degeneracy. Recent experiments under stronger magnetic fields, on the other hand, showed additional plateaus at $\nu = 0, \pm 1, \pm 4$ [2, 3]. Further experiments [4] at $\nu = 0$ in high quality samples revealed a rapid divergence of the longitudinal resistance R_{xx} at a critical field B_c . Interestingly such divergence fits the Kosterlitz-Thouless (KT) [5] form $R_{xx} \sim e^{a/\sqrt{B_c - B}}$ over three decades of the resistance [4]. Moreover, for $B < B_c$ the resistance saturates at low temperature to a value much larger than the quantum of resistance [4], a behavior qualitatively different from conventional thermally activated transport in strong magnetic fields.

Since the critical field B_c lies in the regime where the 4-fold degeneracy of the $N = 0$ Landau levels (LLs) is split, it is important to understand the cause of such splitting. There are several theoretical proposals. The common theme is the observation that the exchange effect of the long-range part of the Coulomb interaction [6] favors the spontaneous polarization of the real and/or valley-spins [7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18]. (the valley-spin is a SU(2) pseudospin variable, which we denote by \mathbf{T} ; its z -component $T_z = +1$ (-1) corresponds to K (K'), respectively.) In one of the proposals, it is argued that the Zeeman energy favors the polarization of the real instead of the valley-spin [11, 12]. In another it is argued that the short-range part of the Coulomb interaction favors the spontaneous polarization of the valley-spin so that K and K' becomes unequally populated [8, 10, 13, 14, 15, 16]. Because the $N = 0$ Landau states associated with K' and K localize on complementary sublattices (A and B , respectively) this amounts to a charge-density-wave (CDW) modulation which breaks the A - B sublattice symmetry.

The type of diverging resistance observed in Ref. [4] is

difficult to account for in the real spin polarization scenario since in this scenario there are spin-filtered counter-propagating edge states that give rise to a metallic conductance of $2e^2/h$ at $\nu = 0$ [11, 12, 19]. Similarly in the CDW scenario [13, 14, 15, 16] it is difficult to explain the KT type resistance divergence, and the high-resistance metallic state below the critical field [4]. In addition to the above, there is a work (Ref. [20]) which claims an explicit valley symmetry breaking term is consistent with the lattice point group symmetry. Like others, this work can not account for the KT behavior.

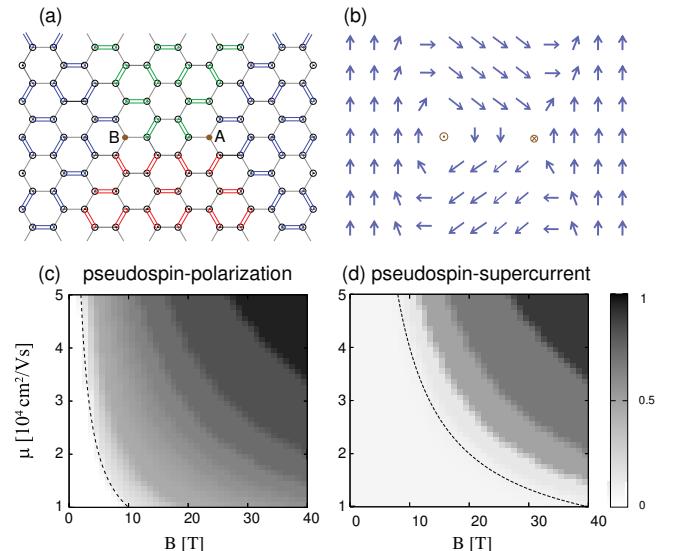


FIG. 1: (Color online) (a) The Kekulé bond-density wave order with two defects marked by a filled circle. The defects are charged as they support a midgap electron state. (b) The $U(1)$ phase $\phi = \tan^{-1}(T_y/T_x)$ corresponding to the bond order pattern (a). (c) The valley-spin polarization ratio as a function of magnetic field B and sample mobility μ . (d) Same as (a) but for the pseudospin-supercurrent $j_{sc}^z/j_{sc}^{z(\text{clean})}$, where $j_{sc}^{z(\text{clean})}$ is the value in the clean limit. The number of orbitals per valley and per spin is $N_\phi = 50$.

Motivated by the KT behavior and the highly resistive metallic state, we propose an alternative scenario: the degeneracy splitting at $\nu = 0$ is due to a spontaneous ordering of the pseudospin on the $T_x - T_y$ plane (XY pseudospin ferromagnet). This involves a spontaneously generated hybridization between the $N = 0$ LLs associated with B (K) and A (K'), and is represented by the ground state wavefunction

$$|\Psi\rangle = \prod_{m,s=\uparrow\downarrow} \frac{1}{\sqrt{2}} \left[c_{Kms}^\dagger + e^{i\phi} c_{K'ms}^\dagger \right] |0\rangle, \quad (1)$$

where $c_{\tau ms}^\dagger$ is the creation operator for an electron in m -th $N = 0$ LL orbital at valley $\tau = K, K'$ with real spin $s = \uparrow, \downarrow$. This type of order also breaks the lattice translation symmetry due to the mixing of B and A , and represents a bond-density-wave of some kind (Kekulé order) [see Fig. 1(a)] [17, 18, 21, 22, 23]. The phase ϕ of this hybridization matrix element is the U(1) phase angle representing the direction in $T_x - T_y$ plane, $\mathbf{T} = (\cos \phi, \sin \phi, 0)$, and associated with the sliding degrees of freedom of this density-wave. The low-energy charged excitations are vortices and antivortices [Fig. 1(b)]. We study their binding-unbinding transition driven by magnetic fields or disorder (see below).

We now take a look at, piece by piece, the Hamiltonian for graphene in a strong magnetic field and the associated energy scales, to address the plausibility of the inter-valley coherent state. (1) At the charge neutral point the LL separation is $\sqrt{2}\hbar v_F/\ell_B \simeq 400\sqrt{B[T]}[K]$, which is the largest energy scale of the problem. Therefore in the rest of the paper we perform projection onto the $N = 0$ LLs.

(2) The Coulomb interaction H_C , which is the second largest energy scale of the problem, is approximately symmetric under rotation in the combined space of real and valley-spins. The exchange energy is $E_C^{\text{ex}} \sim \sqrt{\pi/2}(e^2/\epsilon\ell_B) \simeq 120\sqrt{B[T]}[K]$ [6].

As a result it favors the polarization of the SU(4) spin albeit it does not care whether the polarization should occur in the real spin, or valley-spin, or some combination of both[7].

(3) We now describe the parts of the Hamiltonian which break the SU(4) symmetry, $H_{\text{SB}} = \int d^2r \mathcal{H}_{\text{SB}}$,

$$\mathcal{H}_{\text{SB}} = -\frac{1}{2}\Delta_z S_z - U_0 |\mathbf{S}|^2 - U_z T_z^2 - U_\perp (T_x^2 + T_y^2). \quad (2)$$

Here \mathbf{S} is the real spin operator. The first term in H_{SB} represents the Zeeman energy where $\Delta_z \equiv g\mu_B B \simeq 1.3 \times (B[T])[K]$. The short-range part of the Coulomb interaction is not SU(4) symmetric and gives rise to U_0 and U_z . They can be estimated from the on-site and the nearest neighbor interactions, and are smaller than E_C^{ex} by a factor a/ℓ_B [8, 9], where a is the lattice constant. While U_0 favors the real spin polarization, U_z favors the CDW phase ($T_z \neq 0$) [8, 9, 10].

On the other hand, U_\perp term can arise from the electron-phonon interaction. One such example is the in-plane optical mode at K point, whose interaction with electrons can schematically be represented as [17, 24]

$$H_\perp = f \int d^2r \mathbf{u} \cdot (\psi^\dagger \boldsymbol{\tau} \sigma_x \psi) + \frac{N_C k}{2} \mathbf{u}^2, \quad (3)$$

where $\mathbf{u} = (u_x, u_y)$ represents the (uniform) Kekulé-type distortion of the lattice, k measures the elastic energy, and N_C is the total number of carbon atoms. The two sets of Pauli matrices, $\{\sigma_{x,y,z,0}\}$ and $\{\tau_{x,y,z,0}\}$, act on sublattice (A, B) and valley (K, K'), respectively; $\psi^\dagger(\tau_x \pm i\tau_y)\sigma_x \psi \propto T_x \pm iT_y \propto e^{\pm i\phi}$ serves as the U(1) order-parameter of the Kekulé bond density wave. Upon integrating out the phonon, this give rise to the U_\perp term with $U_\perp \sim 2.0 \times (B[T])[K]$. Note that U_\perp is comparable to Δ_z . This can be traced back to the strong coupling between the K phonon and electrons [25, 26]. Out-of-plane lattice distortion is studied in Ref. [16], and shown to contribute to U_z which are much weaker than that associated with in-plane modes in graphene [24]. The SU(4) breaking terms are summarized in Table I.

Since the SU(4) symmetric part of the Coulomb interaction is much stronger than the symmetry breaking parts H_{SB} it is the former that sets the basic energy scale for the SU(4) symmetry breaking. The symmetry breaking terms simply select the way the SU(4) symmetry is broken: they determine the nature of the ordered phase. Although U_0, U_z, U_\perp in Table I all have similar energy scales, it suggests the U(1) broken inter-valley coherent state (1) is a reasonable candidate for lifting the degeneracy of the $N = 0$ LLs.

We now describe the field-induced transition at zero-temperature using the self-consistent Hartree-Fock (HF) theory. To account for competition between interaction and disorder effects, we allow the XY pseudospin order-parameter to be spatially inhomogeneous. The matrix element of the HF Hamiltonian, in the Landau gauge, can be written in the form [27],

$$\langle m\sigma | H_{\text{HF}} | m'\sigma' \rangle = \sum_{\mathbf{q}} e^{iq_x X_{m'}} \delta_{q_y \ell_B^2, X_m - X_{m'}} \times [U_{\sigma\sigma'}^H(\mathbf{q}) + U_{\sigma\sigma'}^F(\mathbf{q}) + U_{\sigma\sigma'}^{XY}(\mathbf{q}) + \delta_{\sigma\sigma'} U_{\text{imp}}(\mathbf{q})]. \quad (4)$$

Here the system size is $L \times L = 2\pi\ell_B^2 N_\phi$, $X_m = 2\pi\ell_B^2 m/L$

	residual symmetry [(spin) \times (valley)]	energy scale
Δ_z	No \times SU(2)	$1.3[K] \times B[T]$ [3]
U_0	SU(2) \times SU(2)	$1.0[K] \times B[T]$ [8]
U_z	SU(2) $\times \mathbb{Z}_2$ (CDW)	$0.5[K] \times B[T]$ [8]
U_\perp	SU(2) \times U(1) (Kekulé)	$2.0[K] \times B[T]$ [17]

TABLE I: SU(4) symmetry breaking terms, with the pattern of symmetry breaking and the energy scales.

($m = 1, 2, \dots, N_\phi$), and $\sigma = 1, \dots, 4$ is the index for (real)spin and valley. The Hartree and Fock potentials, and the anisotropic interaction are given as follows:

$$\begin{aligned} U_{\sigma\sigma'}^H(\mathbf{q}) &= \frac{\delta_{\sigma\sigma'}}{2\pi\ell_B^2} V_C(\mathbf{q}) e^{-\frac{q^2\ell_B^2}{2}} \sum_{\sigma''} \Delta_{\sigma\sigma''}(\mathbf{q}), \\ U_{\sigma\sigma'}^F(\mathbf{q}) &= -\frac{1}{L^2} \sum_{\mathbf{p}} V_C(\mathbf{p}) e^{-\frac{p^2\ell_B^2}{2} + i\mathbf{q} \times \mathbf{p}\ell_B^2} \Delta_{\sigma\sigma'}(\mathbf{q}), \\ U_{\sigma\sigma'}^{XY}(\mathbf{q}) &= \frac{-U_\perp}{2\pi} \sum_{\sigma_1\sigma_2} \Delta_{\sigma_1\sigma_2}(\mathbf{q}) e^{-\frac{q^2\ell_B^2}{2}} \sum_{j=x,y} \hat{T}_{\sigma\sigma'}^j \hat{T}_{\sigma_1\sigma_2}^j, \end{aligned} \quad (5)$$

where $V_C(\mathbf{q}) = 2\pi e^2/\epsilon q$ and $\hat{T}^j = \sigma_0 \otimes \tau_j$. The SU(4) order-parameter in Eqs. (4, 5) is determined self-consistently from $\Delta_{\sigma'\sigma}(\mathbf{q}) = N_\phi^{-1} \sum_{mm'} \langle c_{m\sigma}^\dagger c_{m'\sigma'} \rangle e^{-iq_x X_m} \delta_{q_y, \ell_B^2, X_{m'} - X_m}$. The disorder potential $U_{\text{imp}}(\mathbf{q})$ is given in terms of charged impurities located randomly at \mathbf{R}_I by $U_{\text{imp}}(\mathbf{q}) = L^{-2} \sum_{I=1}^{N_{\text{imp}}} e^{i\mathbf{q} \cdot \mathbf{R}_I} V_C(\mathbf{q}) e^{-[q^2/4 - iq_x q_y/2]\ell_B^2}$. The disorder strength is described by the impurity filling $\nu_{\text{imp}} = (h/eB)n_{\text{imp}}$, where $n_{\text{imp}} = N_{\text{imp}}/L^2$ is the impurity density. In terms of the zero-field mobility of graphene, $\mu = \sigma_{xx}/ne \simeq 20e/hn_{\text{imp}}$ [7], the disorder strength is determined by a product $B \times \mu$.

In the clean limit, $N_{\text{imp}} = 0$, the ground state is fully pseudospin polarized due to the Coulomb exchange. In a weak field or in a dirty sample, on the other hand, the Coulomb interaction plays a minor role and the four (nearly) degenerated LLs are equally occupied. As shown in Fig. 1 (c), the pseudospin polarization ratio diminishes in the weak field and low mobility limit. In particular when $B < B^* \simeq 10/(\mu[10^4 \text{cm}^2/\text{Vs}])[\text{T}]$ the pseudospin symmetry is restored by disorder. Here B^* , referred to the dashed line in Fig. 1 (c), plays the role of the mean-field critical field.

Even $B > B^*$, vortices and anti-vortices tend to destroy the stiffness of the XY pseudospin order. An inkling of this KT transition could be seen in the unrestricted HF calculation as follows. In the pseudospin XY (quasi-long-range) ordered phase, angle-twisted states which have $\phi = QX_m$ in Eq. (1), namely *pseudospin-supercurrent-flowing states*, are metastable, because of the finite stiffness. Such states can be selected by artificially starting with an initial order-parameter $\Delta_{KK'}(\mathbf{q}) = \delta_{\mathbf{q}, Q\hat{\mathbf{x}}}$ in the initial step of the self-consistency loop. One can then monitor whether or not the pseudospin-supercurrent generated can survive as one iterates the HF calculation[28]. Charged impurities generate quenched vortex-antivortex pairs that randomize ϕ , and hence the pseudospin-supercurrent is expected to vanish in a weak field and low μs (see Fig. 2.) In Fig. 1 (d), the pseudospin-supercurrent of the metastable state, given by [29] $\mathbf{j}_{\text{sc}}^z = \frac{-e}{L^2} \sum_{\mathbf{q}, ss' \tau} \tau [i\mathbf{q} \times \hat{\mathbf{z}}] V_C(\mathbf{q}) \rho_{\tau s}(-\mathbf{q}) \rho_{-\tau s'}(\mathbf{q})$, is plotted, where $\tau = \pm 1$ for K and K' , and $\rho_{\tau s}(\mathbf{q})$ is the density operator for valley τ and spin s . Here note that pseudospin-supercurrents are charge neutral objects

and thus are not related to true charge-currents. We calculate \mathbf{j}_{sc}^z to discriminate whether vortices and antivortices are bound or unbound. As Fig. 1 (d) indicates, the pseudospin supercurrent drops around $B_c \simeq 40/(\mu[10^4 \text{cm}^2/\text{Vs}])[\text{T}] > B^*$.

When $B \gg B_c$ and when the temperatures is sufficiently lower than the Coulomb exchange energy but still finite, the U(1) phase fluctuations are described by the following classical action[5, 6]

$$S_{\text{XY}} = \frac{\rho_s}{2} \int d^2x (\nabla\phi)^2. \quad (6)$$

The unbinding of the vortex-antivortex pairs triggers the KT transition from the pseudo spin XY quasi-long-range ordered phase to the disorder phase at B_c .

Vortices and anti-vortices are charged [6, 23] and they can contribute to electrical transport. The reason why they carry a charge can be understood on the honeycomb lattice as follows [Fig. 1(a)]: A defect in the Kekulé order can be visualized as a A or B sublattice site that is not dimerized with neighbors, and hence supports a midgap state (zero mode). The presence (absence) of an electron on such site makes the Kekulé vortex or antivortex positively (negatively) charged. The pseudo spin is pointing $T_z = +1$ (-1) at the vortex core while $T_z = -1$ ($+1$) at the antivortex core. Hence, the charge and currents generated by vortex excitations are given by $j_\mu = (T_z/\pi) \epsilon_{\mu\nu\lambda} \partial_\nu \partial_\lambda \phi$, where $\mu = 0, x, y$.

In the XY ordered phase where the vortex and antivortex are bound, it is energetically favorable for the T_z of the pair to point in the same direction. As a result, the bound vortex pairs are charge neutral. On the other hand, a charged vortex-antivortex pair can be induced and pinned by charged impurities. As increasing the number of vortex-antivortex pairs, by increasing the impurity density or by decreasing magnetic fields, the binding interactions between vortex and antivortex are screened, causing the KT transition.

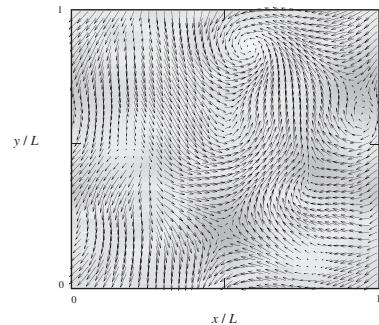


FIG. 2: A typical local XY pseudospin configuration (T_x, T_y) represented by arrows. The z -component is represented by a grey plot with black as $+1$ and white as -1 . The number of orbitals per valley and per spin is $N_\phi = 50$, and the number of impurities is $N_{\text{imp}} = 20$.

In the KT disordered phase ($B^* < B < B_c$), the vortices are unbound, and their diffusion gives rise to a conductivity given by $\sigma \propto n_{\text{vtx}}\mu_{\text{vtx}}$ where n_{vtx} is the density of vortices and μ_{vtx} the mobility. This vortex conducting mechanism is a two-dimensional analog of the soliton conduction mediated by charged defects (domain walls) in polyacetylene[30]. In the KT disordered phase $n_{\text{vtx}} \sim 1/\xi^2$ where ξ is the KT correlation length[5]. Since $\xi \propto e^{a/\sqrt{B_c-B}}$, this gives rise to the KT-divergent resistivity. This argument closely follows the one used by Halperin and Nelson in analyzing the behavior of the electrical conductivity of a thin film superconductor above its KT transition[31]. Indeed, our situation is dual to theirs. In Ref. [31] the Cooper pair (charge) current exerts the magnus force on the vortices and, through the finite vortex mobility, induces a vortex current perpendicular to it. Since vortex current causes an transverse electric field (hence a voltage drop) through the Josephson relation, this gives rise to a finite electrical resistivity. In our case the vortex is charged, and it is the external electric field that induced the vortex (charge) current. Thus our electric field plays the role of charge (Cooper pair) current in Ref. [31], while our charge (vortex) current plays the role of electric field in Ref. [31]. As the result, electrical conductivity in Ref. [31] should be translated into electric resistivity ρ in our case; the finding of $\sigma \sim \xi^2$ in Ref. [31] implies $\rho \sim \xi^2$ in our situation.[32]

The spontaneous inter-valley coherence discussed above is very similar to the inter-layer coherence in the double-layer $\nu = 1$ QHE [6, 33]. However, there are several important differences. (i) The parameter d/ℓ_B (d is the interlayer separation) in the double-layer system is replaced by a/ℓ_B where a is the lattice spacing. For the current system $a/\ell_B \ll 1$, a regime which has not been achieved in the double layer system. (ii) The inter-valley coherent state we propose is spin singlet rather than spin polarized. (From this point of view, the $\nu = 1$ bilayer QH system is similar to the $\nu = \pm 1$ QHE in graphene rather than $\nu = 0$.) Although the (pseudospin) supercurrent cannot be directly measured in the inter-valley coherent state in graphene, these two facts have advantage over double-layer QH systems to observe the KT physics.

We stress that our proposal is motivated by the apparent KT-divergent resistance and the highly resistive metallic state at $\nu = 0$ observed in Ref. [4]. The very basis of our proposal should be subjected to further experimental scrutiny, by changing temperature, magnetic field, doping, and mobility.

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mobility μ_{vtx} , requires the knowledge of detailed dissipation mechanism (in particular, information not included in the electronic part of the problem). In the literature it is usually treated as a phenomenological parameter.

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